

Butane, 1,1,1,2,2,3,3,4,4-nonafluoro-4-methoxy-  
163702-07-6 | DTXSID4073120

## Model Performance

|       |      |
|-------|------|
| Model | Data |
|-------|------|

### Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.87            | 0.81 | 0.87           | 0.82 | 0.86       | 0.86 |

## Model Results

**Predicted value:** 5.60e-03 mol/L

**Global applicability domain:** Outside

**Local applicability domain index:** 3.20e-01

**Confidence level:** 6.06e-01

## Nearest Neighbors from the Training Set

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Chloropentafluoroethane

**Measured:** 3.82e-04

**Predicted:** 7.63e-04

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Ethane, 1,1-dichloro-1,2,2,2-tetrafluoro-

**Measured:** 8.01e-04

**Predicted:** 1.41e-03

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Ethyl 4,4,4-trifluoroacetate

**Measured:** 4.35e-02

**Predicted:** 7.99e-02

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2-Chloro-1,1,1,2-tetrafluoroethane

**Measured:** 1.10e-02

**Predicted:** 8.36e-03

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Diisopropyl fluorophosphate

**Measured:** 8.36e-02

**Predicted:** 8.23e-02